LCA Methodology

Methodology for Developing Gate-to-Gate Life Cycle Inventory Information

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Abstract. Life Cycle Assessment (LCA) methodology evaluates holistically the environmental consequences of a product system or activity, by quantifying the energy and materials used, the wastes released to the environment, and assessing the environmental impacts of those energy, materials and wastes. Despite the international focus on environmental impact and LCA, the quality of the underlying life cycle inventory data is at least as, if not more, important than the more qualitative LCA process.

This work presents an option to generate gate-to-gate life cycle information of chemical substances, based on a transparent methodology of chemical engineering process design (an ab initio approach). In the broader concept of a Life Cycle Inventory (LCI), the information of each gate-to-gate module can be linked accordingly in a production chain, including the extraction of raw materials, transportation, disposal, reuse, etc. to provide a full cradle to gate evaluation. The goal of this article is to explain the methodology rather than to provide a tutorial on the techniques used. This methodology aims to help the LCA practitioner to obtain a fair and transparent estimate of LCI data when the information is not readily available from industry or literature. Results of gate-to-gate life cycle information generated using the cited methodology are presented as a case study.

It has been our experience that both LCI and LCA information provide valuable means of understanding the net environmental consequence of any technology. The LCI information from this methodology can be used more directly in exploring engineering and chemistry changes to improve manufacturing processes. The LCA information can be used to set broader policy and to look at more macro improvements for the environment.

Keywords: Ammonia production; carbon dioxide production; fugitive emissions; gate-to-gate life cycle; heat transfer efficiency; Life Cycle Assessment; Life Cycle Inventory; life cycle of processes; potential energy recovery; process design

Introduction

Life Cycle Assessment (LCA) is a widely accepted tool to evaluate environmental effects of products, processes, and services (SETAC, 1993). The LCA methodology evaluates holistically the environmental consequences of a product system or activity, by quantifying the energy and materials used, the wastes released to the environment, and assessing the potential environmental impacts of those energy, materials, and wastes (Nordic Council, 1995).

A complete life cycle assessment consists of four complementary components: goal and scope definition, inventory analysis, impact assessment, and interpretation (WENZEL, 1997). The backbone of an LCA is a Life Cycle Inventory. The objective of the inventory is to create a model of the product or activity identified during the goal and scope definition.

The collection of data is the most time-consuming part in an LCA and involves a great deal of work to obtain faithful, transparent, and representative information about the many processes in a production system. Quite often, the practitioner faces the frustration of incomplete or missing information.

When performing an LCA of a pharmaceutical or biochemical product, the amount of chemical substances involved in the supply chain increase geometrically in relation of the number of steps in the synthesis. The supply chains in this kind of production networks can reach high degrees of complexity, and therefore, the information available about the chemical substances involved is limited.

Even though the life cycle method is gradually becoming more important for industry to incorporate the environmental factor in processes, services and products, the information about the processes is not readily available. Unfortunately, the substances that are included in the most common LCA databases represent just a part of the raw materials used in chemical and biochemical companies, and it is not easy to obtain the information from the manufacturers due to legal or intellectual property concerns. Frequently the response time from the manufacturers is extremely long, even longer than the time scope for the study.

With that background, the estimation of gate-to-gate life cycle information of chemical substances using chemical engineering process design techniques becomes a feasible and plausible LCI alternative when factual or literature information is not available for a study.

It is a normal practice that the manufacturing plants producing chemical substances use design techniques for such plants, and so no major discrepancies with reality are expected (although not proven) when used for LCI. To further overcome the later concern, the transparency of the methodology and assumptions becomes a priority.

This work presents an option to generate gate-to-gate life cycle information of chemical substances, based in a trans-

parent methodology from chemical engineering process design. In the broader concept of an LCI, the information of each gate-to-gate module can be linked accordingly in a production chain, including the extraction of raw materials, transportation, disposal, reuse, etc.

1 Methodology

The methodology developed for generating gate-to-gate data suitable for creating life cycle information of chemical substances is generated in the following order,

1. **Search and selection of the process.** In this stage the process to be evaluated is chosen. It is important to ensure that the information is as updated as possible, and it is representative of the current industrial practice and of the region under study. The phases of this first stage could be described as follows:

   a) Investigation of the processes that have the greatest industrial importance. Collect all the information regarding the process. Patents, articles, electronic and on-line databases, industrial bulletins, and direct industrial contacts are examples of the sources of information.

   b) Selection of the process to be used. This selection could be based on the amount, age, and scale of the information obtained, as well as on the process that is most common for the regional area under study. For the majority of chemicals there is economic competition that forces a similarity in chemical and energy efficiency. Thus selecting any major process is probably representative, given the modest level of precision needed in complex LCI systems.

2. **Definition of the process.** This second stage determines and delimits the details of the process as such. We seek to define the mass flow of the process, the substances present in the system and the properties, and to identify the reactions involved, and the conditions of all the operations. One decides on components when there is an opportunity of selecting these (e.g. solvents), and determines the unit operations used. The sequence of this stage could be described as follows:

   a) Description of the chemical reactions, including all names and structural formulae for reactants and products.

   b) Identification of the conditions of temperature, pressure and composition under which each operation takes place.

   c) Determination of the reaction conversion and separation efficiencies.

   d) Elaboration of the flow diagram of the process with numbered process streams indicating the temperature and pressure conditions. The utilization of standard symbols is preferred (SANDLER and LUCKIEWICZ, 1987).

   e) Search or estimation of the physical and chemical properties for all direct and indirect chemicals.

3. **Mass Balance.** In this stage, the calculations of inputs and outputs for the process are performed. All materials inputs and outputs will leave or enter the overall manufacturing system at 25° C and 1 atm., unless otherwise required specifically by the conditions of the process. This assures modules can be easily coupled without violating thermodynamic rules. The mass balance results are important from an LCI point of view since

these determine the major contaminants produced in the process. In this stage:

a) A mass balance for a chosen basis of final product is performed. This establishes the general size of the process equipment needed in the design, normally 1,000 kg/h. This design output is intermediate between commodity chemicals and specialized chemicals, since both are included in these LCI calculations (SANDLER and LUCKIEWICZ, 1987). It is also useful to enter in the process diagram every input and output for the overall process. It is also important that an industrial scale be used, so that realistic power and equipment size are used.

b) For estimating the chemical losses, the following are taken into consideration:
   • Any inputs not in the product or marketable by-products are process emissions. Thus mass balances of overall processes are generally achieved. The process emission amounts are defined by variables such as chemical reaction conversion, feasibility of selling by-products, efficiency of the separation processes selected, among others.
   • Material Safety Data Sheets (MSDS) are used for each major process input. This information helps to determine the major impurities entering the system to later estimate, if possible, the fate of these in the manufacturing process.
   • Fugitive losses. The rule of thumb proposed is for any liquid with a boiling point (1 atm.) of 20 to 60°C, assume a 2% fugitive loss. For any liquid with a boiling point (1 atm.) of 60-120°C assume a 1% fugitive loss. For any gases assume a 0.5% fugitive loss. These percentages of fugitive losses are calculated based on the approximate overall amount of chemical present in the manufacturing system, not for each process separately and thus represent the overall manufacturing plant.
   • Any water that is in contact with the other chemicals in the manufacturing process is referred to as contaminated water, and is accounted for separately.

4. **Energy.** The results from this stage will render the amount of energy required from steam, fuel, electricity, and the energy losses of the process. In a further analysis these figures can be the basis for the calculation of the energy-related emissions (using any appropriate factors). Hence the goal is transparency. Important points to take into consideration are:

a) Heat of reaction and heat of dilution.

b) Sensible heat to reach reaction conditions

c) Energy for separation units, which will depend on the separation chosen. The energy for every process is expressed in megajoules (MJ) per 1,000 kg of product in the final state.

d) Energy for materials transportation. For pumps, compressors, fans, blowers, etc., the pressure needed is to transport the fluid a distance of 15 m between individual processes, plus the pressure needed to move the fluid through the next unit process (pressure drop), (WALAS, 1987; WOODS, 1995).

e) For all distillations use a reflux ratio, R = 1.3 (MIX, 1978), showing separately the reboiler energy requirement and the condenser.

f) Potential Energy Recovery. A table is prepared showing all heating requirements (positive) clearly labeled with

the process name. Then all energy losses due to cooling (negative) are added, clearly labeled with the name of the process that is being cooled. Finally, an estimation of how much of this lost energy could be recovered is performed with the efficiency rules shown in **Table 1** (BRANAN, 1994).

Table 1: Heat recovery efficiency

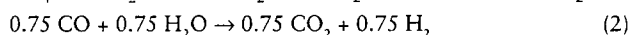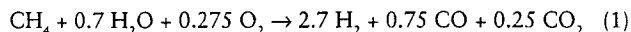| Temperature of Hot Stream Being Cooled	Heat Recovery Efficiency
>500°C	75%
301C-500°C	60%
151C-300°C	45%
60C-150°C	25%
<60°C	0%

2 Results and Discussion

As a case study, the results for the estimation of LCI information for ammonia are presented. Furthermore, those results obtained with the suggested methodology are compared to the values presented by commercially available databases and literature data.

2.1 Estimation of LCI information for ammonia production
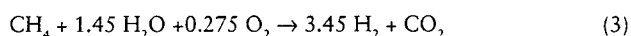
Ammonia is synthesized by a catalytic reaction of hydrogen with nitrogen (Ullmann's, 1997; SLACK, 1973; BRYKOWSKI, 1981; Kirk-Othmer, 1992). The raw materials are a hydrogen source (natural gas, hydrocarbon or coal), air, and water. The process diagram for the ammonia production process is presented in **Fig. 1** where natural gas is used as a hydrogen source, and the synthesis gas is formed by a steam reforming. Carbon dioxide is also produced as a byproduct. The ammonia production process may be divided into the following sub-processes:

A) Synthesis gas preparation

The main goal of this process is to prepare a synthesis gas of nitrogen and hydrogen in the stoichiometric ratio of 1:3. The synthesis gas from natural gas is produced by steam reforming. Carbon monoxide is converted into carbon dioxide in a high/low temperature shift converter.

$$CH_4 + 0.7\ H_2O + 0.275\ O_2 \rightarrow 2.7\ H_2 + 0.75\ CO + 0.25\ CO_2 \quad (1)$$

$$0.75\ CO + 0.75\ H_2O \rightarrow 0.75\ CO_2 + 0.75\ H_2 \quad (2)$$

Overall reaction

$$CH_4 + 1.45\ H_2O + 0.275\ O_2 \rightarrow 3.45\ H_2 + CO_2 \quad (3)$$

B) Carbon dioxide separation/purification

The synthesis gas passes through an absorption tower to separate carbon dioxide before going to the ammonia synthesis process. Removed carbon dioxide is desorbed in a carbon dioxide stripper. The absorbent (such as methylethylamine) is recycled to the absorption tower.

C) Ammonia synthesis

The remaining oxides of carbon in the synthesis gas are removed through a methanation process. The pure synthesis gas is compressed in a steam-turbine centrifugal compressor and combined with the recycled gas. Ammonia is synthesized by the catalytic reaction of hydrogen with nitrogen. Ammonia is refrigerated and separated by a gas/liquid separator.

$$3H_2 + N_2 \rightarrow 2NH_3 \quad (4)$$

The procedure shown in the methodology section was used to estimate the LCI information for ammonia production using process design techniques. A production rate of 1000 kg/hr of ammonia was taken as a basis of the calculations, thus setting the process as an intermediate size ammonia plant. **Table 2** (→ *p. 156*) shows the energy requirements per process unit for ammonia production. The negative energy values in Table 2 represent an energy from process cooling that is recovered to use in heating steam or water. There are two types of the avoided energies – one is an avoided
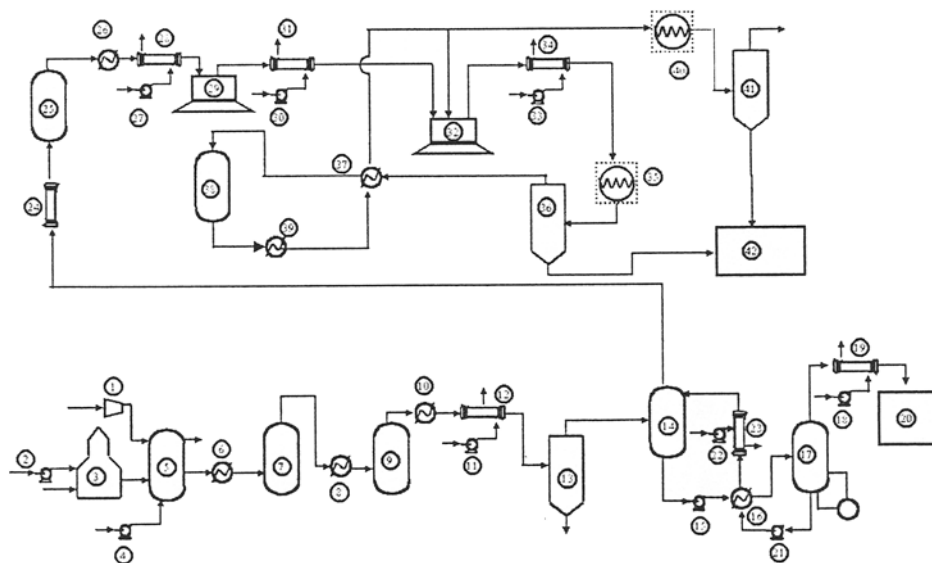

Fig. 1: Process diagram for ammonia manufacturing process. The process operations are indicated in *Table 2*

Table 2: Energy requirement for each unit process and energy recovery

Energy Input (MJ/1000 kg product)			Cooling Requirements (MJ/1000kg product)				
Unit Operation	Energy Input	Cumulative Energy Input	Unit Operation	Energy Loss	Cumulative	Temp. (°C)	Heat Recovered
Compressor A (1)	7.00E+02	7.00E+02	Secondary reformer (5)	-1.27E+03	-1.27E+03	974	-9.50E+02
Pump A (2)	3.46E-03	7.00E+02	Heat recovery A (6)	-3.52E+03	-4.78E+03	974	-3.52E+03
Primary reformer (3)	9.86E+03	1.06E+04	Heat recovery B (8)	-1.38E+03	-6.16E+03	427	-1.38E+03
Pump B (4)	3.42E-02	1.06E+04	Heat recovery C (10)	-2.27E+03	-8.43E+03	266	-1.02E+03
High Temp. Shift converter (7)	-	1.06E+04	Cooler A (12)	-3.37E+02	-8.77E+03	90	-8.41E+01
Low Temp. Shift converter (9)	-	1.06E+04	Cooler B (19)	-5.68E+01	-8.83E+03	82	-1.42E+01
Pump C (11)	4.71E-02	1.06E+04	Cooler C (23)	-2.17E+03	-1.10E+04	80.6	-5.42E+02
Gas/liquid separation (13)	-	1.06E+04	Heat recovery D (26)	-6.84E+02	-1.17E+04	313	-4.10E+02
CO_2 absorber (14)	-	1.06E+04	Cooler D (28)	-3.02E+02	-1.20E+04	121	-7.54E+01
Pump D (15)	4.73E-02	1.06E+04	Cooler E (31)	-1.07E+02	-1.21E+04	177	-4.81E+01
Heat exchanger A (16)	-	1.06E+04	Cooler F (34)	-1.05E+03	-1.31E+04	93	-2.62E+02
CO_2 stripper (17)	2.80E+03	1.34E+04	Heat recovery E (39)	-1.41E+03	-1.45E+04	371	-8.45E+02
Pump E (18)	1.53E-03	1.34E+04					
CO_2 storage tank (20)	-	1.34E+04					
Pump F (21)	4.39E-02	1.34E+04					
Pump G (22)	5.85E-02	1.34E+04					
Heater A (24)	8.96E+02	1.43E+04					
Methanator (25)	3.36E+01	1.43E+04					
Pump H (27)	8.14E-03	1.43E+04					
Steam turbine C. Compressor A (29)	3.37E+03	1.77E+04					
Pump I (30)	2.88E-03	1.77E+04					
Steam turbine C. Compressor B (32)	1.38E+03	1.90E+04					
Pump J (33)	2.83E-02	1.90E+04					
Refrigerator A (35)	3.32E+02	1.94E+04					
Ammonia separator A (36)	-	1.94E+04					
Heat exchanger B (37)	-	1.94E+04					
NH_3 converter (38)	1.80E+02	1.96E+04					
Refrigerator B (40)	4.85E+00	1.96E+04					
Ammonia separator A (41)	-	1.96E+04					
Ammonia storage tank (42)	-	1.96E+04					
Potential energy recovery		-9.15E+03					
Total		1.04E+04	Total recovery				-9.15E+03

energy that is recovered to practically use within a process, and another is a potential avoided energy that is recovered for possible use in heating water or steam.

A summary of the LCI information for this process, including the classification of chemical losses and the estimation of potential heat recovery from the process is presented in Table 3 ($\rightarrow$ p. 157). Energy-related emissions are not documented in Table 3. However, emissions from the combustion of the flue gas, which is recycled within the process, in the primary reformer are taken into account. The energy-related emissions can be easily estimated by energy modules.

2.2 Comparison with other data

It is of interest to check the differences between estimated values and site-specific data. Since the site-specific data are not available up to now, the commercial LCA databases and the literature data are used for comparison. Table 4 ($\rightarrow$ p. 158) presents the inputs, products, and emissions data from Boustead (BOUSTEAD, 1996), PEMS (PIRA, 1998), BUWAL 250 (BUWAL, 1996) and EFMA (EFMA, 1995) for the same process.

In general, it can be said that the methodology works well when compared with different published data and commercially available databases. Most of apparent differences found between the databases and the results given by the methodology seem to be related mainly to the transparency of the data.

Regarding materials, by example, the amounts of natural gas reported by BUWAL and EFMA are in the same range as the results given by this methodology. In the case of Boustead and PEMS, the amount reported includes the natural gas used for fuel. In the proposed methodology, the natural gas used for heating is 364 kg, assuming all the heating comes from steam production using only natural gas. If we add the natural gas used for fuel to the result obtained in the proposed methodology, then the total natural gas in-

Table 3: Summary of Life Cycle Inventory information

Product:	Ammonia
Basis:	1,000 kg/h ammonia
References:	Slack, V.; James, R.G. (1973): Ammonia. Marcel Dekker, Inc.
	Brykowski, F.J. (1981): Ammonia and Synthesis Gas. Noyes Data Corporation
Comments:	All mass and energy units per hour are equivalent to per 1,000 kg of ammonia

Inputs	Amount	Units	Comments
Air	1,796.85	kg/hr	688.6 kg of air is used in burning flue gas
Natural gas	446.75	kg/hr	
Water	1,200	kg/hr	12,000 if cooling water is included with the water used in reaction
Total	3,443.6		

Product	Amount	Units	Comments
Ammonia	1,000	kg/hr	99% purity (9.4 kg/hr water)
Carbon dioxide	1,179	kg/hr	100% purity

Process emissions[a]	Amount				Units	Comments
	Air	Liquid	Solid	Solvent		
Ar	13.29				kg/h	
CH_4	2.23				kg/h	
CO	2.9				kg/h	
CO_2	52.54				kg/h	
H_2	3.07				kg/h	
NH_3	6.42				kg/h	
NO	3.52				kg/h	
NO_2	5.39				kg/h	
Mass balance difference	30.72				kg/h	

Note: Water (513 kg/h), oxygen (27kg/h) and nitrogen (560 kg/h) are not included in this table as process emissions.

Energy Requirements	Amount	Units	Comments
Electricity	7.00E+02	MJ/hr	
Heating – Steam	9.00E+03	MJ/hr	Consider a heat transfer efficiency of 85%
Heating fuel	9.86E+03	MJ/hr	Consider a heat transfer efficiency of 85%
Cooling refrigeration		MJ/hr	
Cooling water	-1.08E+04	MJ/hr	
Potential Heat Recovery	-9.15E+03	MJ/hr	
Net Energy[b]	1.04E+04	MJ/hr	

Notes:
[a] Oxygen and nitrogen are not included.
[b] Energy requirement minus potential heat recovery from cooling systems.
N/A not applicable for this chemical process

cluding fuel and feedstock of 810 kg of natural gas is in the range of the numbers reported by Boustead and PEMS (760 kg of natural gas).

The air inputs are controlled by the stoichiometry of equation (4) and therefore must be on the order of 1,800 kg/1,000 kg ammonia. Thus it is clear that the air inputs in Boustead and PEMS are only of some supplementary part of the overall process (such as the air-activated control systems). The lack of transparency makes this impossible to verify, but the stoichiometry must be closer to the air requirements, as shown in our methodology and EFMA.

There is a clear lack of consistency with regard to the water input, but this may also be just an issue of transparency. The water reported in the NCSU methodology is that required to carry the chemical reaction, and it is in the same range as the data reported by BUWAL and EFMA (920-1,500 kg water/1,000 kg ammonia). This is smaller, by a factor of 10, when compared with Boustead and PEMS. On the other hand, if the cooling water is added to the reacting water (→ *Table 3*, inputs), the value obtained coincides pretty well with the one reported in Boustead and PEMS (11,000-12,000 kg water/1,000 kg ammonia). It is then logical to assume that the latter databases are including cooling water in the total amount of water required and reported. Thus, all five databases may be correct, but are measuring different aspects of water use and, without transparency, the differences are large. These differences would thus have a significant impact on subsequent use of ammonia LCI data.

Reporting products and by-products is also subject to a need for clarity. With the same basis, 1,000 kg of ammonia, the stoichiometry leading to CO_2 is relatively fixed. Three databases chose to identify the carbon dioxide (range, 1,150-1,300 kg/1,000 kg ammonia, → *Table 4*) as a byproduct. However, two other reported the carbon dioxide as an emission.

With use of any one database for the LCI of ammonia, the variability of carbon dioxide emissions is wide, even though the underlying chemistry is similar. In the Boustead and PEMS databases, the reported carbon dioxide emissions are remarkably larger than in the rest of the databases. Applying the reaction stoichiometry (44 kg of carbon dioxide produced by 16 kg of methane) to the total amount of natural gas required reported in these two data sets (760 kg natural gas/1,000 kg of ammonia), which includes both natural gas used for heating and for the reaction, the total carbon dioxide formed was estimated in 2,090 kg CO_2/1,000 kg NH_3, which is similar to the total amount of CO_2 reported. The latter is an indication that the carbon dioxide emissions reported by Boustead and PEMS very likely include the emissions produced during the heating of the processes. On the other hand, the carbon dioxide emission reported in this study is that which is unrecovered by the carbon dioxide byproduct processes, and thus is a residual emission.

Emissions in the case study are the sum of estimated fugitive losses and the estimated emissions from the combustion of the flue gas, which is recycled from an ammonia separation process. Since the fugitive emissions are not normally assessed in production plants, and therefore not reported, the differences in the emissions are most likely attributable to the addi-

Table 4: Comparison of inputs, products and emissions per 1,000 kg of ammonia produced. Data concern only the process for the production of ammonia

Parameter	Case Study	BUWAL 250	Boustead	PEMS	EFMA[d]
Process type	Steam reforming	Steam reforming	n.r.	n.r.	Steam reforming
Inputs					
Natural gas, kg	446.75	467	760 [a]	760 [a]	458
Air, kg	1,796.85	n.r.	5.02	6.6	1,100
Water, kg	1,200 (12,000 [e])	920	11,166	11,000	1,500
Products					
Ammonia, kg	1,000	1,000	1,000	1,000	1,000
CO_2, kg	1,179	1,156	[b]	[b]	1,150 – 1,300
Emissions					
Ar, kg	13.29	n.r	n.r	n.r	n.r
Methane, kg	2.23	7.14	n.r	16 [c]	n.r
CO, kg	2.9	0.025	0.002	0.04 [c]	<0.03
CO_2, kg	52.54	436.1	1,975 [d]	2,055 [d]	500
Non-methane VOC, kg	n.r	0.928	n.r.	n.r.	n.r
Hydrogen, kg	3.07	n.r.	n.r.	n.r.	n.r
Ammonia, kg	6.42	n.r.	0.001	0.001	n.r
NO_x (as NO_2), kg	8.91	0.304	1.17	2.6 [d]	0.6 – 1.3
SO_x (as SO_2), kg	n.r.	0.010	0.036	0.78 [d]	< 0.01

n.r. Not reported
[a] Sum of fuel and feedstock
[b] Reported as emissions
[c] Includes transport emissions. No transport distance is indicated
[d] Emissions are sum of process-related emissions and energy-related emissions
[e] If cooling water is added to reaction water

tional estimation of fugitive emissions, which are normally not measured in many LCI studies or corporate reports. As for carbon dioxide, some data sets treat carbon dioxide formed as an emission, while the case study reported most of it as a byproduct, which is the current industrial practice.

The other larger chemical losses to air are generally 100fold lower than carbon dioxide, hence variability of these reported emissions would be expected to increase. Losses of argon, hydrogen, and ammonia reported in our study, are estimates of fugitive emissions often not reported in regulated permit requirements. The nitrogen oxides are also produced in side reactions. However, there is not SO_x reported since sulfur is largely absent from the process chemistry and the above comparative analysis does not include emissions from heating.

Table 5 shows the energy data available in the databases mentioned above, plus some extra information found in the literature. Total energy requirement in the ammonia manufacturing process ranges from 6,094 MJ to 15,964 MJ. Steam reforming is used in Brykowski's data (BRYKOWSKI, 1981). The energy requirement depends on type of unit process, efficiency of boiler, and efficiency of energy recovery.

The calculations of the energy balance in the case study were reviewed by an industrial person. It was suggested that a

compressor for the natural gas was not required, that 100% efficiency could be applied to the heat recovery A and B, that preheating air at the primary reformer was not necessary, and so on (WEIMER, 1999). Considering his suggestions, the energy requirement decreased by about 20% of the original calculation, and are those listed in Table 5.

Table 5: Comparison energy per 1,000 kg of ammonia produced. Data are only the process for production of ammonia

Parameter	Total Heating [MJ]	Electricity [MJ]	Total Energy [MJ]
Energy			
Case study	12,559	700.15	13,259
BUWAL 250	6,094	n.r.	6,094
PEMS	11,294	320[a]	11,614
Boustead	11,294	330	11,624
EFMA	n.r	n.r	8,000 – 10,000
Brykowski	14,696[b]	475	15,171

n.r. Not reported

[a] Calculated using the European Grid (medium voltage) reported in PEMS
[b] Potential energy recovery rule in this study is adopted to modify the energy calculation for energy recovery within the process

Specific analysis of the total energy separates the needs for electricity and heating of processes and process streams. The design-based methodology yielded an intermediate value for heating, 12,559 MJ/1,000 kg ammonia (databases range, 6,094-14,696 MJ/1,000 kg ammonia). However, we have a higher electricity estimate. Since electricity is only about 4% of the total energy, the influence of the overprediction is of less consequence to total energy requirements.

3 Conclusions

Unfortunately, the substances that are included in the most common LCA databases represent just a part of the raw materials used in chemical and biochemical companies, and it is not easy to obtain the information from the manufacturers due to legal, or intellectual property concerns. Besides, frequently the response time from the manufacturers are extremely long, even longer than the time scope for the study.

Therefore, it is common that the practitioners suffer from incomplete or missing information. This sometimes becomes one of the uncertainty sources in the LCA outcome. Furthermore, it could make LCA practitioners give up the implementation of LCA.

LCI information from the North Carolina State University methodology (ab initio calculations) suggested in this paper is useful to LCA practitioners when the information in both foreground and background system is not available. It can reduce the uncertainty associated with the data gaps.

In general, it was found that the results obtained with the proposed methodology are consistent with the existing information. In the case study for ammonia production, the apparent differences found between this methodology and other databases are mainly due to the degree of transparency of the information presented. Another source of differences is that this methodology includes additional issues that normally are not measured (e.g. fugitive emissions), and therefore these are not likely to be reported in other databases.

The design-based approach using repeatable rules provides very comparable LCI values to the industrial measured information when one examines the large parameters, inputs, by-products, CO_2 emissions and specific energy requirements. An industrial verification correction of about 20% in energy led to the closer results from the design-based approach. However, even without this refinement, the major process emissions and inputs were close to field measurements and energy, within 20%. In the large scale use of LCI information for complex studies, such variation is small compared to having to use zero values because data are unavailable.

Like other methodologies, this one has uncertainties. For instance, the uncertainties may be caused by the choice of efficiency of reactor/separation, the efficiency of boiler/heat transfer, or the choice of process types. Sensitivity analysis however, can overcome those uncertainties.

It also needs to be taken into account that the methodology proposed is intended to be a dynamic tool. The "rules of thumb" here proposed are open to change with the current trends of the industrial production processes, the improvements of process operations, and of pollution prevention methods and technologies (e.g. fugitive emissions). Such changes can be done in a very transparent approach for improvement.

Another merit of this methodology is the identification of the key unit within a process. Since this calculation is a microscopic analysis, it is easily to identify a key unit. Therefore, LCI information from this methodology can be used more directly in exploring engineering and chemistry changes to improve manufacturing processes.

References

BOUSTEAD, I. (1996): Primary Data for Operation. Ammonia Gas Production. No. 3667

BRANAN, C. R. (1994): Rules of Thumb for Chemical Engineers. Gulf Publishing Company

BRYKOWSKI, F.J. (1981): Ammonia and Synthesis Gas. Noyes Data Corporation

BUWAL 250 (1996): Swiss Federal Laboratories for Materials Testing and Research. EMPA, Lerchenfeldstr. 5, CH-9014, St. Gallen

EFMA (1995): Production of Ammonia. European Fertilizer Manufacturer's Association, Brussels, Belgium

KIRK, R.E.; OTHMER, D.F. (1992): Kirk-Othmer Encyclopedia of Chemical technology, 4th ed., John Wiley & Sons

MIX, T.J.; DWECK, J.S.; WEINBERG, M. (1978): CEP [49-55]

Nordic Council of Ministers, Nordic Guidelines on Life Cycle Assessment. (1995): Nordic Council, The Nordic Council

PIRA International (1998): PEMS 4. Randall Road. Leatherhead. Surrey. England

SANDLER, H.J.; LUCKIEWICZ, E.T. (1987): Practical Process Engineering: A Working Approach to Plant Design. XIMIX Inc. Philadelphia, PA, 638p

SLACK, V.; JAMES R.G. (1973): Ammonia. Marcel Dekker, Inc.

Society of Environmental Toxicology and Chemistry (1993): Guidelines for Life Cycle Assessment: A Code of Practice

ULLMANN, F. (1985): Ullmann's Encyclopedia of Industrial Chemistry. 5th ed., John Wiley & Sons

WALAS, S. M.(1987): Chemical Engineering. March 16, [75-81]

WEIMER, R.F.(1999): personal communication

WENZEL, H.; HAUSCHILD, M.; ALTING, L. (1997): Environmental Assessment of Products. Chapman and Hall

WOODS, D.R. (1995): Process Design and Engineering Practice. Prentice Hall